



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 113779

TO: Michael Borin  
Location: Rem 2a55  
Monday, February 23, 2004 *JC 70*  
Art Unit: 1631  
Phone: 272-0713  
Serial Number: 10 / 074679

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### Search Notes

interactions of each **rotamer** with at least part of the rest of the backbone structure to generate OPS, this step including **dead-end elimination (DEE)** computation. Also new are (1) a similar method in which, before defining the **rotamers**, each variable residue is classified as a core, surface or boundary residue; in this case the analysis need not (but preferably does) include **DEE** computation; (2) OPS generated this way; (3) nucleic acid (I) encoding OPS; (4) expression vectors and host cells containing (I); (5) **protein** with a sequence at least 5% different from a known **protein** and being at least 20% more stable; (6) computer-readable memory for this process.

**USE** - The method is used to design **proteins**, e.g. with increased stability or altered biological activity, i.e. the effect of site-directed mutations can be evaluated without having to synthesise the actual **protein**. Typical applications are design of **enzymes** with better heat stability for industrial use in carbohydrate or **protein** processing, and pharmaceutical **proteins** with better thermal and proteolytic stability.

**ADVANTAGE** - Unlike most **protein** design methods, this process is quantitative, allowing lessons to be learnt from earlier design attempts and improving specificity.

Dwg.0/13

FS CPI EPI  
 FA AB  
 MC CPI: B04-E02; B04-E03; B04-E08; B04-F0100E; B04-N04; B11-C08; B12-K04;  
 D05-H09; D05-H12; D05-H14; D05-H17  
 EPI: T01-J15

=> d his

(FILE 'HOME' ENTERED AT 12:59:42 ON 23 FEB 2004)  
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 12:59:52 ON 23 FEB 2004  
 L1 1 S US20020183937/PN  
     E MAYO S/AU  
 L2 138 S E3-E7,E15-E20  
     E BOLON D/AU  
 L3 8 S E3,E5  
 L4 141 S L2,L3  
 L5 26 S L4 AND (BIOCHEM? (L) METHOD?) /SC,SX  
 L6 7 S L4 AND (?PROTOZYM? OR ?ENZYM?)  
 L7 10 S L4 AND ENZYM? /SC,SX

FILE 'REGISTRY' ENTERED AT 13:03:35 ON 23 FEB 2004  
 L8 1 S PROTOZYME/CN  
     E PROTOZYME

FILE 'HCAPLUS' ENTERED AT 13:03:55 ON 23 FEB 2004  
 L9 10 S L8  
 L10 1 S L4 AND L9  
 L11 3 S L6,L7,L10 AND L5  
 L12 33 S L5-L7 NOT L11  
     E COMPUTER/CT  
 L13 37947 S E6+NT OR E11  
 L14 90394 S E19+NT OR E21  
 L15 6365 S E44+NT  
     E E6+ALL  
     E E10+ALL  
 L16 1192 S E4,E5  
     E E7+ALL  
     E E10+ALL

L17 36849 S E4,E3  
 L18 27 S L4 AND L13-L17  
 L19 48 S L4 AND (COMPUT? OR AUTOMAT?)  
 L20 59 S L18,L19,L12  
 L21 44 S L20 AND PROTEIN#/SC,SX,CW  
 L22 15 S L20 NOT L11,L21  
     SEL DN AN 2 3 5 6 7  
 L23 5 S E1-E9  
     SEL DN AN 3 39 44 L21  
 L24 41 S L21 NOT E10-E18  
 L25 46 S L11,L23,L24  
 L26 46 S L25 AND L1-L7,L9-L25  
 L27 12 S L26 AND ROTAMER?  
     E CONFORMATION/CT  
     E E3+ALL  
 L28 108938 S E3-E5  
 L29 1008881 S E1+NT  
 L30 32 S L26 AND L28,L29  
     E SIMULATION/CT  
 L31 280217 S E3,E5,E6+NT  
 L32 265860 S E14+NT  
 L33 29213 S E30,E31  
     E E6+ALL  
 L34 41952 S E3-E5  
 L35 36062 S E2+NT  
 L36 18 S L26 AND L31-L35  
 L37 19 S L27,L36 AND L30  
 L38 27 S L26,L30 NOT L37  
 L39 46 S L37,L38 AND (?ENZYM? OR ?PROTEIN? OR ?PROTOZYM?)  
 L40 9 S L37,L38 AND (PROTEIN? OR ENZYM?)/SC,SX  
 L41 46 S L39,L40  
     E PROTEIN ENGINEERING/CT  
     E E3+ALL  
 L42 3268 S E3  
 L43 139 S L42 AND L13-L17  
 L44 62 S L43 AND L31-L35  
     SEL DN AN L44 13 21 24-27 30 38 40 42 47 49 50 57 62  
 L45 15 S E1-E45  
 L46 57 S L41,L45  
 L47 72 S L43 NOT L44-L46  
 L48 57 S L46 AND L1-L7,L9-L47  
 L49 57 S L48 AND ?PROTEIN?  
 L50 33 S L49 AND 9/SC,SX  
 L51 24 S L49 NOT L50  
 L52 2 S L51 NOT L4  
 L53 35 S L50,L52  
 L54 22 S L49 NOT L53  
 L55 1 S L53,L54 AND INSERT?  
 L56 12 S L53,L54 AND ?MUTAT?  
 L57 3 S L53,L54 AND ACTIVE SITE  
 L58 14 S L53,L54 AND ROTAMER?  
 L59 13 S L53,L54 AND VARIA?  
 L60 33 S L55-L59  
 L61 24 S L53,L54 NOT L60  
     SEL DN AN 5 7 11 13  
 L62 20 S L61 NOT E46-E57  
 L63 53 S L60,L62

FILE 'HCAPLUS' ENTERED AT 13:44:38 ON 23 FEB 2004

FILE 'BIOSIS' ENTERED AT 13:46:25 ON 23 FEB 2004  
     E MAYO S/AU

L64 92 S E3-E9,E24

E BOLON D/AU  
 L65 7 S E3,E4  
 L66 95 S L64,L65  
 L67 18 S L66 AND 00520/CC  
 L68 18 S L66 AND CONFERENCE/DT  
 L69 20 S L66 NOT ARTICLE/DT  
 L70 18 S L67,L68  
     SEL DN AN 3 4 6  
 L71 3 S L70 AND E1-E6  
     E L70 15 ALL

FILE 'BIOSIS' ENTERED AT 13:49:48 ON 23 FEB 2004

FILE 'MEDLINE' ENTERED AT 13:49:58 ON 23 FEB 2004

E MAYO S/AU  
 L72 72 S E3-E10,E19  
     E BOLON D/AU  
 L73 8 S E3,E5,E7  
 L74 76 S L72,L73  
 L75 41 S L74 AND L1./CT  
 L76 44 S L74 AND D12./CT  
 L77 31 S L75 AND L76  
 L78 10 S L75 NOT L77  
     SEL DN AN 2 3 5 8  
 L79 4 S L78 AND E1-E12  
 L80 35 S L77,L79  
 L81 13 S L76 NOT L77-L80  
 L82 28 S L74 NOT L80,L81

FILE 'HCAPLUS, BIOSIS, MEDLINE' ENTERED AT 13:54:27 ON 23 FEB 2004

L83 64 DUP REM L63 L71 L80 (27 DUPLICATES REMOVED)

FILE 'WPIX' ENTERED AT 13:55:40 ON 23 FEB 2004

28647 S G06F019/IC,ICM,ICS  
 L85 1601 S L84 AND G01N033/IC,ICM,ICS  
 L86 488 S L84 AND C12N/IC,ICM,ICS  
 L87 414 S L85 AND L86  
 L88 1 S L87 AND ?PROTOZYM?/BIX  
 L89 122 S (DEE OR (DEAD END OR DEADEND) () ELIMINAT?)/BIX  
 L90 49 S ROTAMER?/BIX  
 L91 11 S L84 AND L89  
 L92 14 S L84 AND L90  
 L93 803 S L84 AND ?PROTEIN?/BIX  
 L94 306 S L84 AND ?ENZYM?/BIX  
 L95 18 S L93,L94 AND L89,L90  
 L96 19 S L91,L92,L95  
 L97 15 S L96 AND L85  
 L98 5 S L96 AND C12N/IC,ICM,ICS  
 L99 19 S L96-L98  
     SEL DN AN 6 11 12 13 14  
 L100 14 S L99 NOT E13-E27  
     SEL DN AN L99 12  
 L101 1 S E28-E30  
     E MAYO S/AU  
 L102 47 S E3-E10  
     E BOLON D/AU  
 L103 1 S E3,E5  
 L104 10 S L84 AND L102,L103  
 L105 9 S L104 NOT SPREADSHEET/TI  
 L106 17 S L88,L100,L101,L105 AND L84-L105

FILE 'WPIX' ENTERED AT 14:15:19 ON 23 FEB 2004